

Hydrogen cyanide
74-90-8 | DTXSID9024148

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 36.1 °C

Global applicability domain: Outside

Local applicability domain index: 4.74e-01

Confidence level: 5.64e-01

Nearest Neighbors from the Training Set

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Hydrogen cyanide

Measured: 25.6

Predicted: 36.1

Image not found

Methyl isocyanide

Measured: 59.6

Predicted: 49.3

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Trimethylamine

Measured: 2.87

Predicted: 19.3

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Nitromethane

Measured: 101

Predicted: 90.5

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Acetaldehyde oxime

Measured: 115

Predicted: 110